

Linear Chain of Coupled Quantum Dots

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A linearly coupled chain of spin-polarized quantum dots is investigated under the condition that the number of electrons is equal to or less than the number of the dots. The chemical potential of the system, $\mu_N = E(N) - E(N-1)$, satisfies, $(\mu_N + \mu_{N_\ell+2-N})/2 \approx V + 2t$ ($N, N_\ell, V, E(N)$ and t are the number of electrons, the number of dots, and the strength of nearest neighbor electron-electron interactions, the total groundstate energy and the hopping integral between two adjacent dots). This property will be reflected in the spacing between the conductance peaks. The electron density structures are determined using a quantum Monte Carlo method. As the number of electrons is varied several correlated structures are found that are commensurate/incommensurate with the periodic dot system. Hartree-Fock theory fails to predict the correct electronic structures of this system because several nearly degenerate solutions exist.

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Recent advances in nano-fabrication techniques have made it possible to make quantum dots [1,2]. These structures have several similarities to atoms and are called artificial atoms. The physical parameters of these systems may be controlled easily: the electron density can be varied significantly by the substrate voltage V_g and the range of electron-electron interactions can be controlled by changing the distance to the metallic layer. When these artificial atoms are coupled structures similar to a molecule may arise. Recently numerous groups have started to investigate whether coupled two-dot systems really have molecular properties. Properties of a two-dot system have been studied both experimentally [3-7] and theoretically [8,9]. When many dots are coupled an artificial one-dimensional crystal may be created. It is possible to couple up to ten or more dots together since the size of the total system can be made smaller than the phase coherence length. Such a system has energy bands separated by energy gaps, and transport properties of such a periodic crystal have been investigated experimentally [10].

When the length of such a periodic crystal is infinite the system exhibits many intriguing properties. Depending of the values of the physical parameters the system can have properties of a Luttinger liquid or a generalized Wigner crystal [11]. It is unclear whether these properties remain in a finite system of coupled dots. The purpose of this paper is to examine general properties of a linear chain of spin-polarized dots under the condition $N \leq N_\ell$. We find the following properties. The chemical potential of the system satisfies, $(\mu_N + \mu_{N_\ell+2-N})/2 \approx V + 2t$. This property of the chemical potential is reflected in the spacing between the con-

ductance peaks [12]. The electron density structures, determined by a quantum Monte Carlo method, show several types of commensurate/incommensurate structures as the number of electrons is varied. The groundstate electronic properties of these structures cannot be described by mean field theory (Hartree-Fock theory) except for a few isolated cases. The reason for this failure is the existence of many nearly degenerate solutions.

As shown by recent experiments when $N \leq N_\ell$ the system can be easily spin-polarized [10]. The Hamiltonian of such a coupled dots is given by [13]

$$\begin{aligned} H &= H_t + H_V \\ &= -t \sum_{i=1}^{N_\ell-1} (c_{i+1}^+ c_i + c_i^+ c_{i+1}) + 2tN \\ &\quad + V \sum_{i=1}^{N_\ell-1} n_i n_{i+1} \end{aligned} \quad (1)$$

The operator $c_i(c_i^+)$ destroys (creates) an electron in the i -th dot. The term $2tN$ allows to measure single particle energies from zero.

The presence of the end sites at 1 and N_ℓ breaks particle-hole symmetry. However, the system can be mapped into a ring of $(N_\ell + 1)$ -coupled dots by imposing the periodic boundary condition $c_{N_\ell+2} = c_1$ and requiring the electron occupation number at the site $N_\ell + 1$ to be zero:

$$H = -t \sum_{i=1}^{N_\ell+1} (c_{i+1}^+ c_i + c_i^+ c_{i+1})$$

$$+V \sum_{i=1}^{N_\ell+1} n_i n_{i+1} + w_{N_\ell+1} n_{N_\ell+1} + 2tN. \quad (2)$$

When the strength of the impurity potential energy, $w_{N_\ell+1}$, is large and positive the occupation number at the site $N_\ell + 1$ will be zero. We rewrite the Hamiltonian using the hole creation and hole occupation number operators $h_i^+ = c_i$ and $m_i = 1 - n_i$:

$$H = H' + (V + 2t)(2N - N_\ell - 1), \quad (3)$$

where

$$\begin{aligned} H' = & t \sum_{i=1}^{N_\ell+1} (h_{i+1}^+ h_i + h_i^+ h_{i+1}) \\ & + V \sum_{i=1}^{N_\ell+1} m_i m_{i+1} \\ & + w_{N_\ell+1} (1 - m_{N_\ell+1}) + 2tN_h. \end{aligned} \quad (4)$$

The quantity N_h is the total number of holes, equal to $N_\ell + 1 - N$. From this transformation we find the relation

$$E(N) = E'(N_\ell + 1 - N) + (V + 2t)(2N - N_\ell - 1), \quad (5)$$

where $E(N)$ is the groundstate energy of H with N electrons, and $E'(N)$ denotes the counterpart of H' . For sufficiently large N_ℓ the impurity contributions to the groundstate energies are negligible in both H and H' , and we may set

$$E'(N) \approx E(N) \quad (6)$$

From this it follows

$$(\mu_N + \mu_{N_\ell+2-N})/2 \approx V + 2t. \quad (7)$$

For comparison it should be noted that complete electron-hole symmetry of a ring of N_ℓ dots leads to

$$(\mu_N + \mu_{N_\ell+1-N})/2 = V + 2t. \quad (8)$$

Note that the second subscript in Eq. (8) contains 1 instead of 2. In a finite linear chain or in the presence of disorder this relation is not valid because electron-hole symmetry is broken.

We have solved Eq. (1) by a Hartree-Fock method. The ground state is determined by the following equations

$$H_{HF}|k\rangle = \epsilon_k|k\rangle \quad (9)$$

Here the Hartree-Fock Hamiltonian is given by

$$\begin{aligned} H_{HF} = & -t \sum_{i=1}^{N_\ell-1} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + \sum_{i=1}^{N_\ell} X_i c_i^\dagger c_i \\ & - V \sum_{i=1}^{N_\ell-1} \langle n_{i+1} \rangle \langle n_i \rangle. \end{aligned} \quad (10)$$

where

$$X_i = V(\langle n_{i+1} \rangle + \langle n_{i-1} \rangle).$$

The electron density $\{\langle n_i \rangle\}$ and the Hartree-Fock eigenstates $\{|k\rangle\}$ should be determined self-consistently. Note that $\langle n_0 \rangle = \langle n_{N_\ell+1} \rangle = 0$. The total energy of N -electron system is given in terms of the Hartree-Fock eigenstates $\{|k\rangle\}$:

$$E(N) = \sum_{k=1}^N \epsilon_k - \frac{1}{2} \sum_{k,q=1}^N (\langle kq|H_V|kq\rangle - \langle kq|H_V|qk\rangle), \quad (11)$$

where

$$\begin{aligned} \langle kq|H_V|kq\rangle &= 2V \sum_{i=1}^{N_\ell-1} |a_i(k)|^2 |a_{i+1}(q)|^2, \\ \langle kq|H_V|qk\rangle &= 2V \sum_{i=1}^{N_\ell-1} a_i(k)^* a_i(q) a_{i+1}(k)^* a_{i+1}(q). \end{aligned}$$

The amplitude of the k th eigenstate at site i is $a_i(k)$.

Fig. 1 displays the lowest HF solutions for an odd value of $N_\ell = 7$. Since they have nearly degenerate energies we must include quantum fluctuations to find the true groundstate. Fig. 2 displays the density profiles obtained using a quantum Monte Carlo method [14]. We used typically 500 000 - 1 000 000 Monte Carlo steps to measure the values and the statistical error is about the size of the symbols. Quantum Monte Carlo and HF results differ significantly. The HF theory overestimates the repulsive interactions, and consequently favors structures with more oscillations. A commensurate structure is found at $N = 4$. Generally, when N_ℓ is odd a commensurate state exists for $N = (N_\ell + 1)/2$. This type of states have interesting optical properties [11]. Quantum Monte Carlo results show that the number of peaks is equal to N when $N \leq N_\ell/2$. The number of minima is equal to $N_\ell - N$ for $N > N_\ell/2$.

Fig. 3 displays quantum Monte Carlo density profiles for an even value of $N_\ell = 14$. In both cases the following structures are present: $(\bullet, \bullet, \circ, \bullet, \bullet, \circ), (\circ, \circ, \bullet, \circ, \bullet, \circ, \bullet)$ where the symbols \bullet and \circ denote relatively large and small occupation numbers. HF or classical theory fails to predict these structures. Note that when $N_\ell/N > 1/2$ the occupation number increases as the site index moves away from the center and the values of n_i are large at $i = 1$ and N_ℓ . This is because the electrons feel strong mutual repulsion. The opposite is true for $N_\ell/N < 1/2$. Note that, in contrast to infinite systems, the groundstates do not resemble a liquid state even for $V = 1$. Generally when N_ℓ is even a commensurate (periodic) state is absent, since two classically degenerate state exists. Again we note that the number of peaks is N when

$N \leq N_\ell/2$, and the number of minima is $N_\ell - N$ when $N > N_\ell/2$.

The inset in Fig. 4 displays N versus μ_N for $N_\ell = 15$ and $V = 4$. The distance between the $(N + 1)$ -th and N -th peaks is equal to $\mu_{N+1} - \mu_N$ [12]. The constant charging model would fail to account for these results since the separations between the peaks are not a constant. We have tested the accuracy of Eq. (7) numerically by plotting $(\mu_N + \mu_{N_\ell+2-N})/2$ as a function of N . We see in Fig. 5 that even for small N_ℓ Eq. (7) is well satisfied.

Kouwenhoven *et al.* [10] have shown that their experimental data are better described by assuming presence of some disorder. We have also carried out a similar calculation in the presence of an impurity, and find that our result is in qualitative agreement with that of Kouwenhoven *et al.* [15] It would be interesting to test the validity of Eq. (5) experimentally in a clean coupled-dot system without impurities. Strong correlation effects should be more visible in conductance positions the larger the ratio V/t is. A finite chain of linearly coupled quantum dots is well suited for observing both commensurate/incommensurate electronic structures.

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FIG. 1. Occupation numbers, n_i , as a function of site index, i . The three lowest energy states of a Hartree-Fock calculation are plotted. The strength of nearest-neighbor electron-electron interactions, the electron number, and the number of dots are $V = 5$, $N = 3$, and $N_\ell = 7$. Here the energies are measured in units of t . The graphs are shifted vertically for the sake of clarity of display.

FIG. 2. Quantum Monte Carlo results of occupation numbers for six different electron numbers N . The parameters are $V = 5$ and $N_\ell = 7$.

FIG. 3. Quantum Monte Carlo results of occupation numbers for nine different electron numbers N . The solid lines are for $V = 4$ while dotted lines are for $V = 1$. The total site number is $N_\ell = 14$.

FIG. 4. Chemical potential, μ_N , measured in unit of t is plotted as a function of N . Results for (N_ℓ, V) equal to $(15,4)$, $(14,4)$, and $(14,1)$ are represented by circles, inverted triangles, and triangles. The inset displays N versus μ_N for $(N_\ell, V) = (15, 4)$. The energy difference between two adjacent values of μ_N corresponds to the spacing between two nearby conductance peaks.

FIG. 5. The quantity $(\mu_N + \mu_{N_\ell+2-N})/2$, measured in unit of t is plotted as a function of N to test whether it is approximately equal to a constant $V + 2t$. Results for (N_ℓ, V) equal to $(15,4)$, $(14,4)$, $(14,1)$, $(7,4)$, and $(7,1)$ are represented by circles, inverted triangles, and triangles, diamonds, and squares.









